



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:04 AM UTC

PDB ID : 2YO1 / pdb_00002yo1
Title : Salmonella enterica SadA 1049-1304 fused to GCN4 adaptors (SadAK9- cII)
Authors : Hartmann, M.D.; Hernandez Alvarez, B.; Lupas, A.N.
Deposited on : 2012-10-20
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

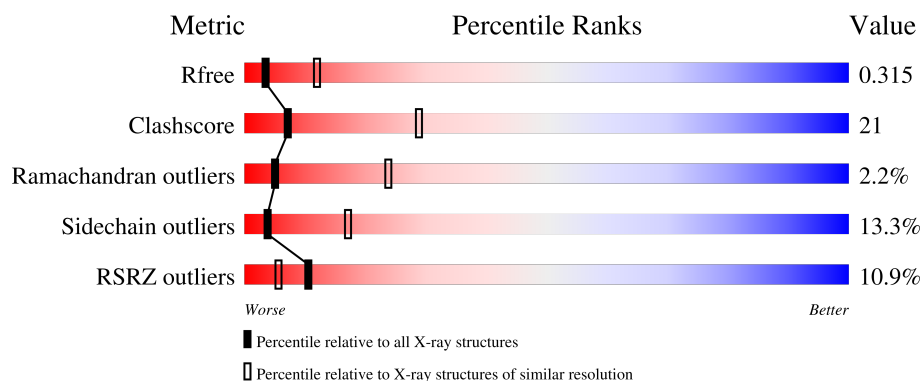
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	322	7% 52% 27% 5% 15%
1	B	322	12% 52% 28% • 15%
1	C	322	9% 49% 30% 5% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5775 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GENERAL CONTROL PROTEIN GCN4, PUTATIVE INNER MEMBRANE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			1929	1159	347	418	5			
1	B	273	Total	C	N	O	S	0	0	0
			1919	1157	344	414	4			
1	C	273	Total	C	N	O	S	0	0	0
			1926	1152	348	421	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1023	ILE	LEU	engineered mutation	UNP Q8ZL64
A	1027	ILE	VAL	engineered mutation	UNP Q8ZL64
A	1030	ILE	LEU	engineered mutation	UNP Q8ZL64
A	1034	ILE	ASN	engineered mutation	UNP Q8ZL64
A	1037	ILE	LEU	engineered mutation	UNP Q8ZL64
A	1041	ILE	VAL	engineered mutation	UNP Q8ZL64
A	1044	ILE	LEU	engineered mutation	UNP Q8ZL64
A	1048	ILE	VAL	engineered mutation	UNP Q8ZL64
A	1308	ILE	LEU	engineered mutation	UNP P03069
A	1312	ILE	VAL	engineered mutation	UNP P03069
A	1315	ILE	LEU	engineered mutation	UNP P03069
A	1319	ILE	ASN	engineered mutation	UNP P03069
A	1322	ILE	LEU	engineered mutation	UNP P03069
A	1326	ILE	VAL	engineered mutation	UNP P03069
A	1329	ILE	LEU	engineered mutation	UNP P03069
A	1333	ILE	VAL	engineered mutation	UNP P03069
A	1334	LYS	-	expression tag	UNP Q8ZL64
A	1335	LEU	-	expression tag	UNP Q8ZL64
A	1336	HIS	-	expression tag	UNP Q8ZL64
A	1337	HIS	-	expression tag	UNP Q8ZL64
A	1338	HIS	-	expression tag	UNP Q8ZL64
A	1339	HIS	-	expression tag	UNP Q8ZL64

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1340	HIS	-	expression tag	UNP Q8ZL64
A	1341	HIS	-	expression tag	UNP Q8ZL64
B	1023	ILE	LEU	engineered mutation	UNP Q8ZL64
B	1027	ILE	VAL	engineered mutation	UNP Q8ZL64
B	1030	ILE	LEU	engineered mutation	UNP Q8ZL64
B	1034	ILE	ASN	engineered mutation	UNP Q8ZL64
B	1037	ILE	LEU	engineered mutation	UNP Q8ZL64
B	1041	ILE	VAL	engineered mutation	UNP Q8ZL64
B	1044	ILE	LEU	engineered mutation	UNP Q8ZL64
B	1048	ILE	VAL	engineered mutation	UNP Q8ZL64
B	1308	ILE	LEU	engineered mutation	UNP P03069
B	1312	ILE	VAL	engineered mutation	UNP P03069
B	1315	ILE	LEU	engineered mutation	UNP P03069
B	1319	ILE	ASN	engineered mutation	UNP P03069
B	1322	ILE	LEU	engineered mutation	UNP P03069
B	1326	ILE	VAL	engineered mutation	UNP P03069
B	1329	ILE	LEU	engineered mutation	UNP P03069
B	1333	ILE	VAL	engineered mutation	UNP P03069
B	1334	LYS	-	expression tag	UNP Q8ZL64
B	1335	LEU	-	expression tag	UNP Q8ZL64
B	1336	HIS	-	expression tag	UNP Q8ZL64
B	1337	HIS	-	expression tag	UNP Q8ZL64
B	1338	HIS	-	expression tag	UNP Q8ZL64
B	1339	HIS	-	expression tag	UNP Q8ZL64
B	1340	HIS	-	expression tag	UNP Q8ZL64
B	1341	HIS	-	expression tag	UNP Q8ZL64
C	1023	ILE	LEU	engineered mutation	UNP Q8ZL64
C	1027	ILE	VAL	engineered mutation	UNP Q8ZL64
C	1030	ILE	LEU	engineered mutation	UNP Q8ZL64
C	1034	ILE	ASN	engineered mutation	UNP Q8ZL64
C	1037	ILE	LEU	engineered mutation	UNP Q8ZL64
C	1041	ILE	VAL	engineered mutation	UNP Q8ZL64
C	1044	ILE	LEU	engineered mutation	UNP Q8ZL64
C	1044	ILE	VAL	engineered mutation	UNP Q8ZL64
C	1308	ILE	LEU	engineered mutation	UNP P03069
C	1312	ILE	VAL	engineered mutation	UNP P03069
C	1315	ILE	LEU	engineered mutation	UNP P03069
C	1319	ILE	ASN	engineered mutation	UNP P03069
C	1322	ILE	LEU	engineered mutation	UNP P03069
C	1326	ILE	VAL	engineered mutation	UNP P03069
C	1329	ILE	LEU	engineered mutation	UNP P03069
C	1333	ILE	VAL	engineered mutation	UNP P03069

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1334	LYS	-	expression tag	UNP Q8ZL64
C	1335	LEU	-	expression tag	UNP Q8ZL64
C	1336	HIS	-	expression tag	UNP Q8ZL64
C	1337	HIS	-	expression tag	UNP Q8ZL64
C	1338	HIS	-	expression tag	UNP Q8ZL64
C	1339	HIS	-	expression tag	UNP Q8ZL64
C	1340	HIS	-	expression tag	UNP Q8ZL64
C	1341	HIS	-	expression tag	UNP Q8ZL64

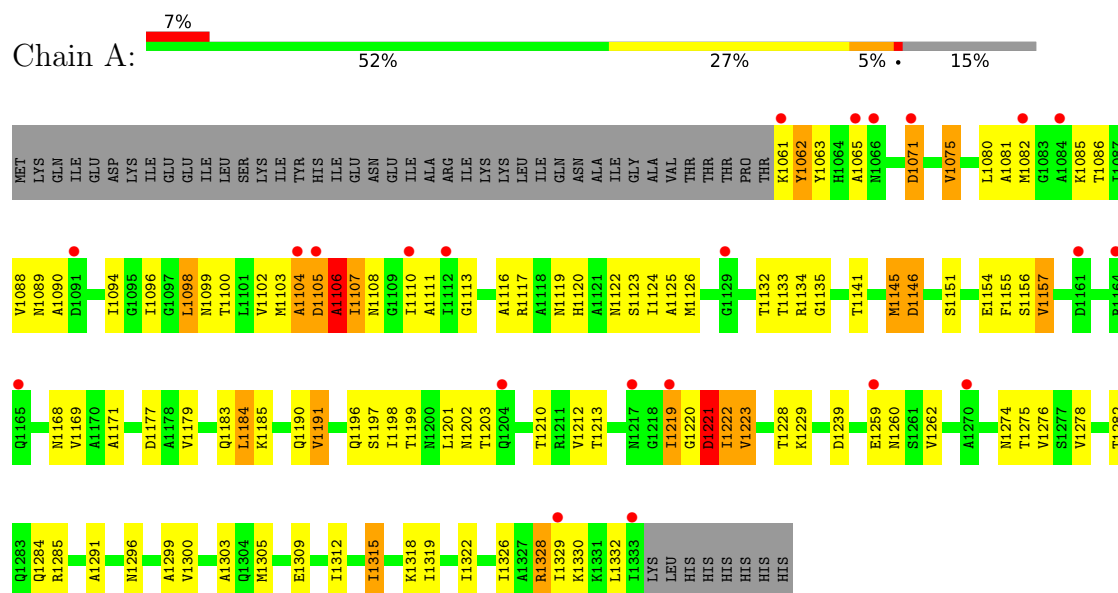
- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Cl 1 1	0	0

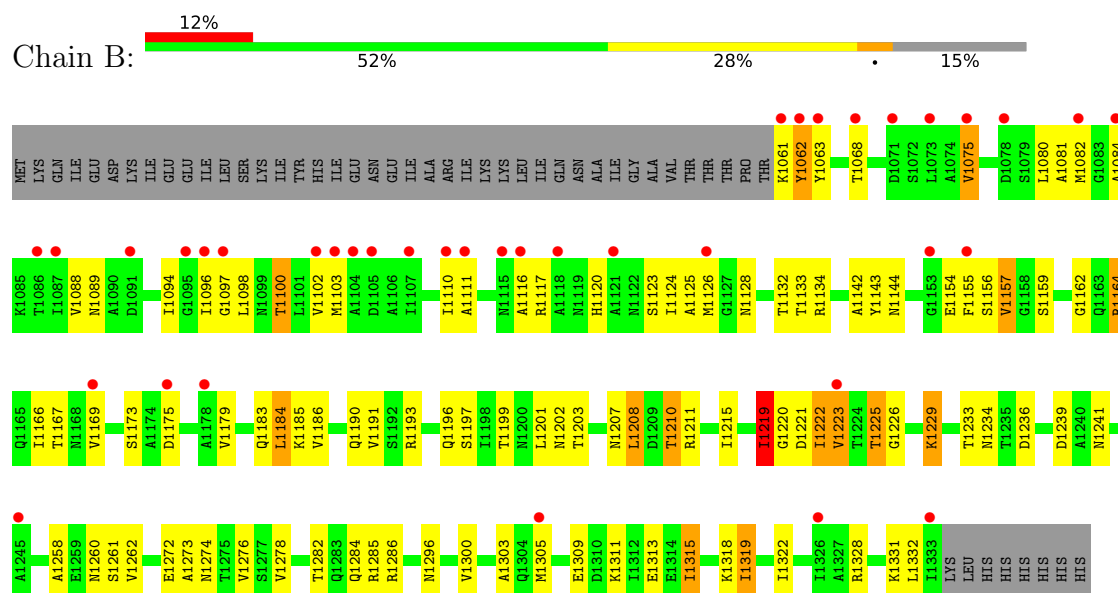
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

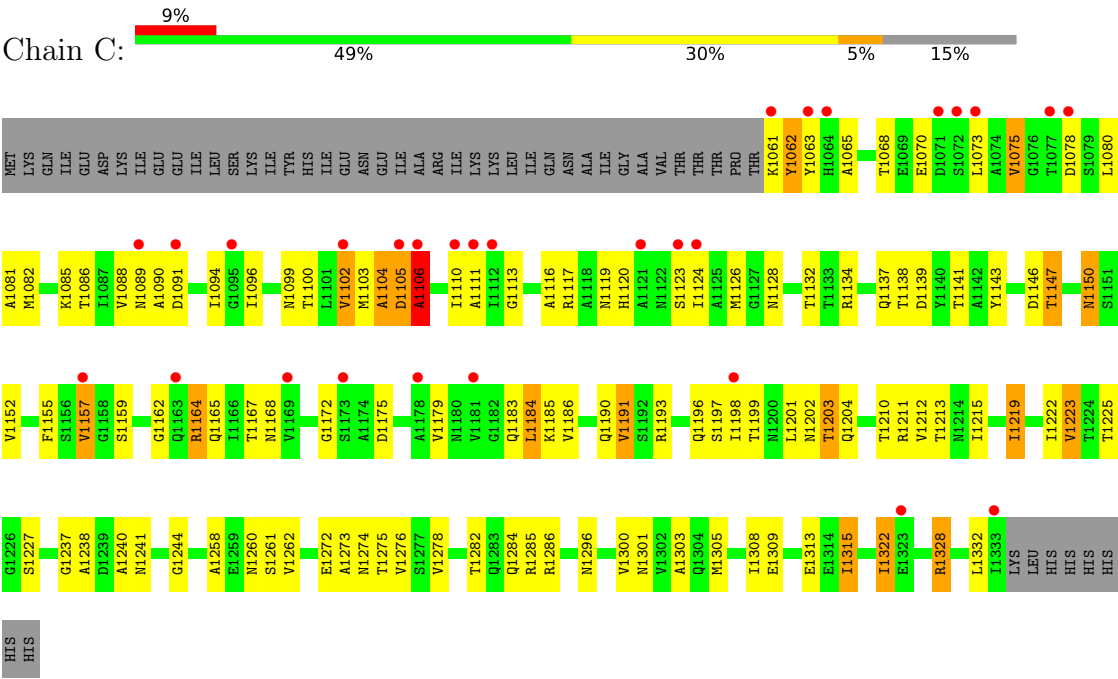
- Molecule 1: GENERAL CONTROL PROTEIN GCN4, PUTATIVE INNER MEMBRANE PROTEIN



- Molecule 1: GENERAL CONTROL PROTEIN GCN4, PUTATIVE INNER MEMBRANE PROTEIN



● Molecule 1: GENERAL CONTROL PROTEIN GCN4, PUTATIVE INNER MEMBRANE PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.03Å 48.78Å 135.83Å 90.00° 105.10° 90.00°	Depositor
Resolution (Å)	38.64 – 3.10 38.64 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.0 (38.64-3.10) 97.1 (38.64-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.265 , 0.320 0.270 , 0.315	Depositor DCC
R_{free} test set	974 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5775	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.88	2/1940 (0.1%)	0.97	2/2641 (0.1%)
1	B	0.89	0/1930	1.01	4/2628 (0.2%)
1	C	0.88	0/1936	1.00	2/2637 (0.1%)
All	All	0.88	2/5806 (0.0%)	0.99	8/7906 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1291	ALA	CA-CB	-6.80	1.42	1.53
1	A	1299	ALA	CA-CB	-5.01	1.45	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1315	ILE	CB-CA-C	-5.83	104.50	111.97
1	C	1164	ARG	N-CA-C	5.40	118.25	108.69
1	B	1169	VAL	N-CA-C	5.32	115.52	107.75
1	A	1169	VAL	N-CA-C	5.23	115.39	107.75
1	C	1315	ILE	CB-CA-C	-5.21	105.30	111.97
1	B	1164	ARG	N-CA-C	5.20	117.90	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1315	ILE	CB-CA-C	-5.06	105.49	111.81
1	B	1225	THR	N-CA-C	5.04	118.69	112.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1106	ALA	Peptide
1	C	1106	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1929	0	1840	97	0
1	B	1919	0	1830	95	0
1	C	1926	0	1823	123	0
2	C	1	0	0	0	0
All	All	5775	0	5493	234	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (234) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1201:LEU:HD11	1:B:1202:ASN:OD1	1.43	1.15
1:A:1124:ILE:HD13	1:C:1126:MET:CE	1.77	1.14
1:A:1124:ILE:CD1	1:C:1126:MET:HE3	1.78	1.13
1:A:1126:MET:HE3	1:B:1124:ILE:HD13	1.30	1.11
1:A:1090:ALA:HB3	1:A:1102:VAL:HG11	1.45	0.99
1:C:1090:ALA:HB3	1:C:1102:VAL:HG11	1.46	0.97
1:B:1219:ILE:HG22	1:B:1220:GLY:N	1.80	0.96
1:B:1126:MET:HE3	1:C:1124:ILE:HD13	1.45	0.95
1:A:1124:ILE:HD13	1:C:1126:MET:HE3	0.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:MET:O	1:A:1104:ALA:O	1.89	0.91
1:A:1107:ILE:HG23	1:A:1108:ASN:HB2	1.53	0.90
1:C:1103:MET:O	1:C:1104:ALA:O	1.89	0.89
1:B:1305:MET:HE3	1:B:1309:GLU:OE2	1.71	0.88
1:C:1090:ALA:CB	1:C:1102:VAL:HG11	2.04	0.87
1:B:1219:ILE:CG2	1:B:1220:GLY:N	2.36	0.86
1:B:1219:ILE:HG22	1:B:1220:GLY:H	1.38	0.84
1:A:1202:ASN:OD1	1:C:1201:LEU:HD11	1.78	0.83
1:A:1278:VAL:O	1:A:1285:ARG:HD2	1.79	0.83
1:A:1315:ILE:HG21	1:C:1315:ILE:HD13	1.60	0.82
1:A:1094:ILE:HD13	1:C:1096:ILE:HG22	1.61	0.82
1:B:1278:VAL:O	1:B:1285:ARG:HD2	1.81	0.80
1:C:1278:VAL:O	1:C:1285:ARG:HD2	1.84	0.78
1:A:1111:ALA:HB1	1:A:1116:ALA:HB1	1.66	0.77
1:C:1305:MET:HE3	1:C:1309:GLU:OE2	1.86	0.76
1:B:1219:ILE:HD12	1:C:1223:VAL:HG23	1.66	0.76
1:A:1126:MET:CE	1:B:1124:ILE:HD13	2.13	0.75
1:B:1201:LEU:CD2	1:C:1201:LEU:HB3	2.18	0.74
1:A:1090:ALA:CB	1:A:1102:VAL:HG11	2.18	0.73
1:A:1126:MET:HE3	1:B:1124:ILE:CD1	2.13	0.73
1:A:1100:THR:HG22	1:A:1113:GLY:O	1.88	0.72
1:A:1305:MET:HE3	1:A:1309:GLU:OE2	1.90	0.72
1:C:1081:ALA:HB2	1:C:1088:VAL:HG21	1.71	0.72
1:C:1111:ALA:HB1	1:C:1116:ALA:HB1	1.69	0.72
1:B:1111:ALA:HB1	1:B:1116:ALA:HB1	1.69	0.72
1:B:1081:ALA:HB2	1:B:1088:VAL:HG21	1.74	0.70
1:C:1134:ARG:HD2	1:C:1137:GLN:HE21	1.56	0.70
1:A:1061:LYS:O	1:A:1062:TYR:HB2	1.92	0.70
1:C:1073:LEU:HG	1:C:1075:VAL:HG23	1.73	0.69
1:A:1104:ALA:O	1:A:1106:ALA:N	2.27	0.68
1:B:1167:THR:HG22	1:C:1134:ARG:NH2	2.09	0.67
1:B:1219:ILE:CD1	1:C:1223:VAL:HG23	2.24	0.67
1:C:1090:ALA:CB	1:C:1102:VAL:CG1	2.73	0.67
1:C:1203:THR:HG22	1:C:1204:GLN:N	2.08	0.67
1:A:1090:ALA:HB3	1:A:1102:VAL:CG1	2.23	0.67
1:B:1061:LYS:O	1:B:1062:TYR:HB2	1.94	0.67
1:A:1090:ALA:CB	1:A:1102:VAL:CG1	2.74	0.66
1:B:1233:THR:HG23	1:B:1233:THR:O	1.95	0.66
1:C:1061:LYS:O	1:C:1062:TYR:HB2	1.96	0.66
1:A:1145:MET:HE2	1:B:1186:VAL:HG21	1.78	0.65
1:B:1296:ASN:HB3	1:C:1303:ALA:HB2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1296:ASN:HB3	1:B:1303:ALA:HB2	1.78	0.65
1:B:1201:LEU:HD11	1:C:1202:ASN:OD1	1.96	0.65
1:B:1219:ILE:O	1:B:1222:ILE:HB	1.98	0.64
1:C:1134:ARG:HD2	1:C:1137:GLN:NE2	2.13	0.64
1:A:1086:THR:HG23	1:A:1100:THR:OG1	1.98	0.63
1:B:1210:THR:HG22	1:B:1211:ARG:N	2.13	0.63
1:C:1090:ALA:HB2	1:C:1102:VAL:CG1	2.29	0.63
1:C:1104:ALA:O	1:C:1106:ALA:N	2.33	0.62
1:B:1098:LEU:HD11	1:C:1078:ASP:HB3	1.81	0.62
1:C:1081:ALA:HB2	1:C:1088:VAL:CG2	2.29	0.62
1:C:1086:THR:HG23	1:C:1100:THR:OG1	2.01	0.61
1:A:1094:ILE:CD1	1:C:1096:ILE:HG22	2.30	0.60
1:A:1081:ALA:HB2	1:A:1088:VAL:HG21	1.84	0.60
1:B:1167:THR:HG22	1:C:1134:ARG:CZ	2.31	0.60
1:A:1096:ILE:HG22	1:B:1094:ILE:HD13	1.82	0.60
1:C:1222:ILE:N	1:C:1222:ILE:HD12	2.17	0.59
1:B:1081:ALA:HB2	1:B:1088:VAL:CG2	2.32	0.59
1:A:1303:ALA:HB2	1:C:1296:ASN:HB3	1.85	0.58
1:B:1222:ILE:HG22	1:B:1223:VAL:N	2.18	0.58
1:B:1222:ILE:O	1:B:1226:GLY:N	2.36	0.58
1:A:1104:ALA:O	1:A:1105:ASP:C	2.47	0.58
1:A:1312:ILE:HD11	1:C:1308:ILE:HG23	1.85	0.58
1:A:1262:VAL:HB	1:A:1276:VAL:HG13	1.85	0.58
1:A:1219:ILE:HG23	1:C:1219:ILE:HD11	1.86	0.58
1:B:1111:ALA:HB1	1:B:1116:ALA:CB	2.35	0.57
1:B:1063:TYR:CZ	1:C:1063:TYR:HB3	2.38	0.57
1:C:1111:ALA:HB1	1:C:1116:ALA:CB	2.34	0.57
1:A:1219:ILE:HD11	1:B:1219:ILE:HG13	1.86	0.57
1:B:1219:ILE:CD1	1:C:1219:ILE:HG23	2.35	0.57
1:A:1094:ILE:HD13	1:C:1096:ILE:CG2	2.32	0.57
1:B:1219:ILE:HD13	1:C:1219:ILE:HG23	1.88	0.56
1:C:1219:ILE:HA	1:C:1222:ILE:HD13	1.86	0.56
1:B:1123:SER:OG	1:B:1132:THR:HG21	2.06	0.56
1:B:1126:MET:CE	1:C:1124:ILE:HD13	2.29	0.56
1:C:1100:THR:HG22	1:C:1113:GLY:O	2.07	0.55
1:A:1260:ASN:HD22	1:A:1274:ASN:HD22	1.52	0.55
1:A:1312:ILE:CD1	1:C:1308:ILE:HG23	2.36	0.55
1:B:1084:ALA:HB3	1:B:1098:LEU:HD23	1.89	0.55
1:B:1102:VAL:HG12	1:B:1102:VAL:O	2.07	0.55
1:B:1133:THR:H	1:B:1154:GLU:CD	2.14	0.55
1:B:1211:ARG:O	1:B:1215:ILE:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:ALA:HB1	1:A:1116:ALA:CB	2.34	0.54
1:B:1097:GLY:O	1:B:1100:THR:HG23	2.08	0.54
1:C:1241:ASN:C	1:C:1241:ASN:OD1	2.50	0.54
1:A:1094:ILE:O	1:A:1110:ILE:HA	2.08	0.54
1:B:1126:MET:HE3	1:C:1124:ILE:CD1	2.27	0.54
1:A:1085:LYS:O	1:A:1099:ASN:HA	2.07	0.54
1:B:1159:SER:N	1:B:1162:GLY:O	2.40	0.54
1:A:1104:ALA:O	1:A:1106:ALA:HB3	2.08	0.54
1:A:1184:LEU:HD12	1:B:1143:TYR:HE2	1.72	0.54
1:A:1120:HIS:CE1	1:A:1134:ARG:HA	2.44	0.53
1:A:1201:LEU:HD23	1:B:1201:LEU:HB3	1.90	0.53
1:B:1260:ASN:HD22	1:B:1274:ASN:HD22	1.56	0.53
1:B:1258:ALA:O	1:B:1261:SER:OG	2.22	0.53
1:C:1104:ALA:O	1:C:1105:ASP:C	2.51	0.53
1:B:1075:VAL:HG11	1:B:1089:ASN:HD22	1.74	0.53
1:B:1120:HIS:CE1	1:B:1134:ARG:HA	2.44	0.53
1:A:1081:ALA:HB2	1:A:1088:VAL:CG2	2.38	0.52
1:C:1260:ASN:HD22	1:C:1274:ASN:HD22	1.57	0.52
1:A:1156:SER:OG	1:C:1168:ASN:ND2	2.39	0.52
1:C:1102:VAL:HG12	1:C:1102:VAL:O	2.09	0.52
1:C:1328:ARG:O	1:C:1332:LEU:HD13	2.09	0.52
1:C:1184:LEU:O	1:C:1185:LYS:C	2.52	0.52
1:A:1201:LEU:CD2	1:B:1201:LEU:HB3	2.40	0.52
1:C:1120:HIS:CE1	1:C:1134:ARG:HA	2.45	0.51
1:A:1065:ALA:CB	1:B:1080:LEU:HD23	2.41	0.51
1:B:1096:ILE:HG22	1:C:1094:ILE:HD13	1.93	0.51
1:C:1146:ASP:O	1:C:1147:THR:HG23	2.10	0.51
1:A:1123:SER:OG	1:A:1132:THR:HG21	2.10	0.50
1:A:1198:ILE:HD13	1:C:1197:SER:HB2	1.92	0.50
1:A:1222:ILE:HD13	1:A:1222:ILE:N	2.27	0.50
1:C:1159:SER:N	1:C:1162:GLY:O	2.43	0.50
1:A:1063:TYR:OH	1:C:1080:LEU:HD22	2.11	0.50
1:A:1065:ALA:HB2	1:B:1080:LEU:CD2	2.42	0.50
1:B:1315:ILE:HD13	1:C:1315:ILE:HG21	1.93	0.49
1:C:1203:THR:CG2	1:C:1204:GLN:N	2.75	0.49
1:C:1075:VAL:HG11	1:C:1089:ASN:HD22	1.77	0.49
1:C:1219:ILE:O	1:C:1222:ILE:N	2.43	0.49
1:B:1201:LEU:HD23	1:C:1201:LEU:HB3	1.90	0.49
1:C:1094:ILE:O	1:C:1110:ILE:HA	2.13	0.49
1:C:1211:ARG:O	1:C:1215:ILE:HD13	2.13	0.49
1:A:1104:ALA:C	1:A:1106:ALA:N	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:ILE:CD1	1:C:1322:ILE:HG23	2.43	0.49
1:A:1065:ALA:HB2	1:B:1080:LEU:HD23	1.94	0.48
1:B:1184:LEU:HD12	1:C:1143:TYR:HE2	1.78	0.48
1:C:1272:GLU:O	1:C:1273:ALA:C	2.56	0.48
1:A:1090:ALA:HB2	1:A:1102:VAL:CG1	2.42	0.48
1:A:1124:ILE:HG22	1:A:1125:ALA:N	2.29	0.48
1:A:1075:VAL:HG11	1:A:1089:ASN:HD22	1.79	0.48
1:C:1155:PHE:CE1	1:C:1157:VAL:HG13	2.48	0.48
1:C:1278:VAL:O	1:C:1285:ARG:CD	2.58	0.48
1:A:1102:VAL:O	1:A:1102:VAL:HG12	2.13	0.48
1:A:1105:ASP:O	1:A:1106:ALA:C	2.56	0.48
1:A:1155:PHE:CE1	1:A:1157:VAL:HG13	2.49	0.48
1:A:1326:ILE:HD12	1:C:1322:ILE:HG23	1.96	0.48
1:C:1150:ASN:OD1	1:C:1150:ASN:N	2.47	0.48
1:B:1211:ARG:NH2	1:C:1212:VAL:HG12	2.29	0.48
1:C:1104:ALA:O	1:C:1106:ALA:HB3	2.14	0.48
1:A:1190:GLN:O	1:A:1191:VAL:C	2.55	0.48
1:B:1262:VAL:HB	1:B:1276:VAL:HG13	1.96	0.47
1:C:1105:ASP:O	1:C:1106:ALA:C	2.57	0.47
1:A:1315:ILE:HD13	1:B:1315:ILE:HG21	1.94	0.47
1:C:1222:ILE:HD12	1:C:1222:ILE:H	1.78	0.47
1:A:1155:PHE:HE2	1:C:1126:MET:HE2	1.79	0.47
1:A:1103:MET:O	1:A:1104:ALA:C	2.57	0.47
1:A:1229:LYS:NZ	1:B:1223:VAL:O	2.47	0.47
1:B:1142:ALA:HB1	1:C:1172:GLY:O	2.14	0.47
1:B:1221:ASP:O	1:B:1225:THR:HG23	2.15	0.47
1:A:1328:ARG:O	1:A:1332:LEU:HD13	2.15	0.47
1:A:1145:MET:CE	1:B:1186:VAL:HG21	2.44	0.46
1:A:1145:MET:O	1:A:1146:ASP:HB2	2.15	0.46
1:C:1198:ILE:HG22	1:C:1202:ASN:HD21	1.80	0.46
1:A:1315:ILE:CG2	1:C:1315:ILE:HD13	2.36	0.46
1:C:1103:MET:SD	1:C:1119:ASN:ND2	2.88	0.46
1:B:1100:THR:HB	1:B:1116:ALA:HB3	1.98	0.46
1:B:1155:PHE:CE1	1:B:1157:VAL:HG13	2.49	0.46
1:A:1126:MET:CE	1:B:1124:ILE:HG21	2.46	0.45
1:C:1179:VAL:HG22	1:C:1183:GLN:HB2	1.97	0.45
1:A:1212:VAL:HG12	1:C:1211:ARG:NH2	2.31	0.45
1:B:1166:ILE:HG23	1:C:1155:PHE:HD1	1.81	0.45
1:C:1085:LYS:O	1:C:1099:ASN:HA	2.16	0.45
1:A:1080:LEU:HD23	1:C:1065:ALA:HB2	1.98	0.45
1:A:1133:THR:H	1:A:1154:GLU:CD	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1175:ASP:OD1	1:C:1185:LYS:NZ	2.45	0.45
1:B:1201:LEU:HD21	1:C:1201:LEU:HB3	1.99	0.44
1:C:1203:THR:O	1:C:1204:GLN:C	2.59	0.44
1:A:1098:LEU:HD12	1:A:1098:LEU:H	1.82	0.44
1:A:1201:LEU:HB3	1:C:1201:LEU:HD23	1.99	0.44
1:B:1286:ARG:HB2	1:C:1275:THR:HG22	2.00	0.44
1:A:1220:GLY:O	1:A:1221:ASP:C	2.60	0.44
1:B:1094:ILE:O	1:B:1110:ILE:HA	2.17	0.44
1:C:1103:MET:O	1:C:1104:ALA:C	2.59	0.44
1:A:1103:MET:HB2	1:A:1119:ASN:HA	2.00	0.44
1:A:1171:ALA:HB1	1:A:1183:GLN:CD	2.43	0.44
1:A:1135:GLY:HA2	1:A:1154:GLU:HB3	2.00	0.43
1:A:1122:ASN:CG	1:C:1128:ASN:ND2	2.77	0.43
1:B:1144:ASN:O	1:C:1186:VAL:HG11	2.18	0.43
1:B:1179:VAL:HG22	1:B:1183:GLN:HB2	2.00	0.43
1:B:1128:ASN:N	1:B:1164:ARG:HH22	2.16	0.43
1:C:1104:ALA:C	1:C:1106:ALA:N	2.76	0.43
1:B:1124:ILE:HG22	1:B:1125:ALA:N	2.33	0.43
1:B:1162:GLY:HA3	1:C:1152:VAL:HG21	2.01	0.43
1:C:1128:ASN:HD22	1:C:1164:ARG:NH2	2.17	0.43
1:A:1134:ARG:NH2	1:C:1167:THR:HG22	2.34	0.42
1:A:1168:ASN:ND2	1:B:1156:SER:OG	2.50	0.42
1:A:1179:VAL:HG22	1:A:1183:GLN:HB2	2.00	0.42
1:B:1219:ILE:HD13	1:C:1219:ILE:CG2	2.49	0.42
1:C:1301:ASN:OD1	1:C:1301:ASN:C	2.62	0.42
1:C:1225:THR:OG1	1:C:1227:SER:HB2	2.18	0.42
1:A:1103:MET:SD	1:A:1119:ASN:ND2	2.93	0.42
1:B:1190:GLN:HA	1:B:1193:ARG:HH11	1.85	0.42
1:A:1177:ASP:CG	1:C:1134:ARG:HH22	2.27	0.42
1:C:1123:SER:OG	1:C:1132:THR:HG21	2.20	0.42
1:B:1157:VAL:O	1:B:1164:ARG:CD	2.68	0.42
1:B:1184:LEU:O	1:B:1185:LYS:C	2.63	0.42
1:B:1233:THR:O	1:B:1233:THR:CG2	2.64	0.42
1:C:1258:ALA:O	1:C:1261:SER:OG	2.31	0.42
1:C:1081:ALA:CB	1:C:1088:VAL:CG2	2.97	0.42
1:C:1190:GLN:HA	1:C:1193:ARG:HH11	1.85	0.42
1:B:1234:ASN:ND2	1:C:1244:GLY:O	2.50	0.42
1:A:1185:LYS:NZ	1:C:1175:ASP:OD1	2.51	0.42
1:A:1259:GLU:OE1	1:A:1260:ASN:HB2	2.19	0.41
1:A:1278:VAL:O	1:A:1285:ARG:CD	2.59	0.41
1:B:1167:THR:CG2	1:C:1134:ARG:CZ	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:ILE:O	1:A:1330:LYS:C	2.63	0.41
1:B:1272:GLU:O	1:B:1273:ALA:C	2.63	0.41
1:B:1328:ARG:O	1:B:1332:LEU:HD13	2.20	0.41
1:A:1179:VAL:HG13	1:C:1179:VAL:HG12	2.01	0.41
1:C:1262:VAL:HB	1:C:1276:VAL:HG13	2.03	0.41
1:B:1229:LYS:O	1:C:1240:ALA:N	2.52	0.41
1:C:1141:THR:HG23	1:C:1141:THR:O	2.21	0.41
1:A:1275:THR:HA	1:C:1286:ARG:O	2.21	0.41
1:B:1208:LEU:HD23	1:C:1212:VAL:HG21	2.03	0.41
1:C:1070:GLU:HG2	1:C:1085:LYS:HG2	2.02	0.41
1:A:1071:ASP:N	1:A:1071:ASP:OD1	2.53	0.41
1:A:1197:SER:O	1:A:1201:LEU:HD13	2.21	0.41
1:A:1318:LYS:HD2	1:B:1319:ILE:HG21	2.03	0.41
1:B:1173:SER:N	1:C:1165:GLN:HE22	2.18	0.41
1:B:1197:SER:HB2	1:C:1198:ILE:HD13	2.03	0.41
1:B:1241:ASN:OD1	1:B:1241:ASN:C	2.64	0.41
1:C:1190:GLN:O	1:C:1191:VAL:C	2.64	0.41
1:B:1207:ASN:O	1:B:1208:LEU:C	2.65	0.40
1:C:1237:GLY:O	1:C:1238:ALA:C	2.64	0.40
1:C:1128:ASN:ND2	1:C:1164:ARG:NH2	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/322 (84%)	236 (87%)	26 (10%)	9 (3%)	3	17
1	B	271/322 (84%)	235 (87%)	32 (12%)	4 (2%)	8	32
1	C	271/322 (84%)	238 (88%)	28 (10%)	5 (2%)	6	28
All	All	813/966 (84%)	709 (87%)	86 (11%)	18 (2%)	5	24

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1062	TYR
1	A	1104	ALA
1	A	1105	ASP
1	B	1062	TYR
1	C	1062	TYR
1	C	1104	ALA
1	C	1105	ASP
1	A	1106	ALA
1	A	1145	MET
1	A	1146	ASP
1	B	1103	MET
1	B	1219	ILE
1	B	1239	ASP
1	C	1106	ALA
1	A	1098	LEU
1	A	1223	VAL
1	A	1221	ASP
1	C	1147	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/257 (77%)	172 (86%)	27 (14%)	3	16
1	B	195/257 (76%)	168 (86%)	27 (14%)	3	15
1	C	198/257 (77%)	173 (87%)	25 (13%)	4	19
All	All	592/771 (77%)	513 (87%)	79 (13%)	4	17

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1071	ASP
1	A	1075	VAL
1	A	1082	MET

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Mol	Chain	Res	Type
1	A	1107	ILE
1	A	1117	ARG
1	A	1141	THR
1	A	1151	SER
1	A	1157	VAL
1	A	1184	LEU
1	A	1191	VAL
1	A	1196	GLN
1	A	1199	THR
1	A	1203	THR
1	A	1210	THR
1	A	1213	THR
1	A	1219	ILE
1	A	1221	ASP
1	A	1222	ILE
1	A	1223	VAL
1	A	1228	THR
1	A	1239	ASP
1	A	1282	THR
1	A	1284	GLN
1	A	1300	VAL
1	A	1319	ILE
1	A	1322	ILE
1	A	1328	ARG
1	B	1068	THR
1	B	1075	VAL
1	B	1082	MET
1	B	1100	THR
1	B	1117	ARG
1	B	1157	VAL
1	B	1184	LEU
1	B	1191	VAL
1	B	1196	GLN
1	B	1199	THR
1	B	1203	THR
1	B	1208	LEU
1	B	1210	THR
1	B	1219	ILE
1	B	1222	ILE
1	B	1223	VAL
1	B	1229	LYS
1	B	1236	ASP

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Mol	Chain	Res	Type
1	B	1282	THR
1	B	1284	GLN
1	B	1300	VAL
1	B	1311	LYS
1	B	1313	GLU
1	B	1318	LYS
1	B	1319	ILE
1	B	1322	ILE
1	B	1331	LYS
1	C	1068	THR
1	C	1075	VAL
1	C	1082	MET
1	C	1091	ASP
1	C	1102	VAL
1	C	1117	ARG
1	C	1138	THR
1	C	1139	ASP
1	C	1150	ASN
1	C	1157	VAL
1	C	1184	LEU
1	C	1191	VAL
1	C	1196	GLN
1	C	1199	THR
1	C	1203	THR
1	C	1210	THR
1	C	1213	THR
1	C	1219	ILE
1	C	1223	VAL
1	C	1282	THR
1	C	1284	GLN
1	C	1300	VAL
1	C	1313	GLU
1	C	1322	ILE
1	C	1328	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1089	ASN
1	A	1196	GLN
1	A	1207	ASN
1	A	1260	ASN

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Mol	Chain	Res	Type
1	A	1283	GLN
1	A	1296	ASN
1	B	1089	ASN
1	B	1207	ASN
1	B	1260	ASN
1	B	1267	ASN
1	B	1283	GLN
1	C	1089	ASN
1	C	1115	ASN
1	C	1137	GLN
1	C	1165	GLN
1	C	1168	ASN
1	C	1196	GLN
1	C	1202	ASN
1	C	1207	ASN
1	C	1260	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	273/322 (84%)	0.75	22 (8%) 18 10	20, 65, 119, 151	0
1	B	273/322 (84%)	0.87	38 (13%) 6 4	20, 65, 137, 168	0
1	C	273/322 (84%)	0.78	29 (10%) 11 6	20, 69, 129, 142	0
All	All	819/966 (84%)	0.80	89 (10%) 10 5	20, 66, 131, 168	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1105	ASP	8.2
1	B	1178	ALA	6.9
1	B	1111	ALA	5.7
1	B	1169	VAL	5.7
1	C	1077	THR	5.5
1	B	1096	ILE	5.0
1	C	1091	ASP	5.0
1	A	1112	ILE	4.9
1	B	1061	LYS	4.1
1	B	1095	GLY	4.1
1	A	1217	ASN	4.0
1	C	1061	LYS	4.0
1	C	1071	ASP	3.9
1	B	1105	ASP	3.8
1	C	1333	ILE	3.8
1	B	1087	ILE	3.5
1	B	1118	ALA	3.4
1	B	1110	ILE	3.4
1	B	1082	MET	3.2
1	A	1165	GLN	3.2
1	C	1111	ALA	3.2
1	C	1078	ASP	3.1
1	C	1063	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	1173	SER	3.1
1	A	1065	ALA	3.1
1	C	1072	SER	3.0
1	C	1102	VAL	3.0
1	B	1086	THR	3.0
1	A	1082	MET	3.0
1	B	1107	ILE	3.0
1	B	1071	ASP	3.0
1	C	1110	ILE	3.0
1	B	1104	ALA	2.9
1	C	1106	ALA	2.9
1	A	1204	GLN	2.9
1	A	1329	ILE	2.8
1	A	1219	ILE	2.8
1	A	1333	ILE	2.8
1	B	1155	PHE	2.8
1	C	1124	ILE	2.7
1	B	1075	VAL	2.7
1	C	1095	GLY	2.7
1	A	1104	ALA	2.7
1	C	1073	LEU	2.7
1	A	1105	ASP	2.6
1	A	1084	ALA	2.6
1	B	1068	THR	2.6
1	A	1270	ALA	2.6
1	C	1181	VAL	2.5
1	A	1061	LYS	2.5
1	C	1178	ALA	2.5
1	B	1175	ASP	2.5
1	B	1073	LEU	2.5
1	C	1157	VAL	2.5
1	B	1121	ALA	2.5
1	C	1123	SER	2.5
1	C	1198	ILE	2.5
1	C	1064	HIS	2.4
1	B	1223	VAL	2.4
1	B	1084	ALA	2.4
1	B	1097	GLY	2.4
1	C	1112	ILE	2.3
1	A	1259	GLU	2.3
1	B	1333	ILE	2.3
1	B	1245	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1126	MET	2.3
1	B	1062	TYR	2.3
1	C	1163	GLN	2.3
1	C	1089	ASN	2.3
1	A	1071	ASP	2.2
1	A	1161	ASP	2.2
1	B	1116	ALA	2.2
1	B	1063	TYR	2.2
1	B	1103	MET	2.2
1	B	1326	ILE	2.2
1	C	1121	ALA	2.2
1	A	1129	GLY	2.2
1	A	1164	ARG	2.2
1	C	1169	VAL	2.1
1	B	1305	MET	2.1
1	B	1078	ASP	2.1
1	B	1102	VAL	2.1
1	B	1153	GLY	2.1
1	A	1066	ASN	2.0
1	A	1091	ASP	2.0
1	B	1091	ASP	2.0
1	A	1110	ILE	2.0
1	B	1115	ASN	2.0
1	C	1323	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	C	2334	1/1	0.88	0.22	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.